



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2024 – 02:40 PM EDT

PDB ID : 1KT2  
Title : CRYSTAL STRUCTURE OF CLASS II MHC MOLECULE IEK BOUND TO MOTH CYTOCHROME C PEPTIDE  
Authors : Fremont, D.H.; Dai, S.; Chiang, H.; Crawford, F.; Marrack, P.; Kappler, J.  
Deposited on : 2002-01-15  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

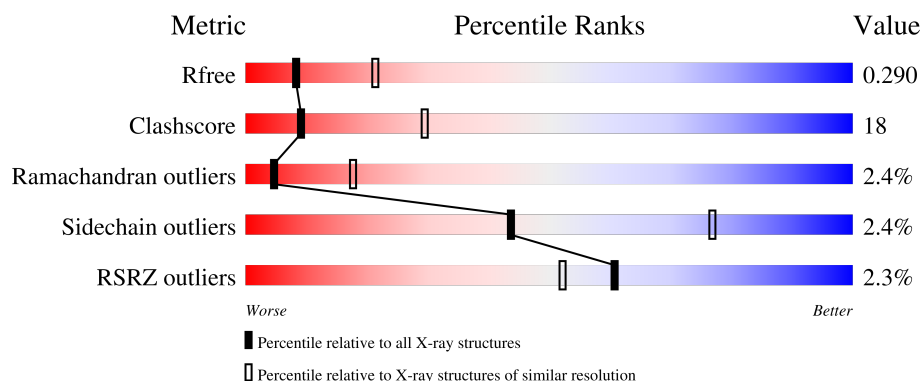
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	182	<div> <div>0%</div> <div>69%</div> <div>29%</div> <div>•</div> </div>
1	C	182	<div> <div>70%</div> <div>27%</div> <div>•</div> </div>
2	B	213	<div> <div>5%</div> <div>65%</div> <div>33%</div> <div>•</div> </div>
2	D	213	<div> <div>3%</div> <div>55%</div> <div>43%</div> <div>•</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	E	2	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6743 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called H-2 class II histocompatibility antigen, E-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1500	965	245	286	4			
1	C	182	Total	C	N	O	S	0	0	0
			1500	965	245	286	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	HIS	THR	SEE REMARK 999	UNP P01904
C	177	HIS	THR	SEE REMARK 999	UNP P01904

- Molecule 2 is a protein called Fusion protein consisting of cytochrome C peptide, glycine rich linker, and MHC E-beta-k.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	99	0	0
			1722	1090	299	327	6			
2	D	213	Total	C	N	O	S	77	0	0
			1722	1090	299	327	6			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

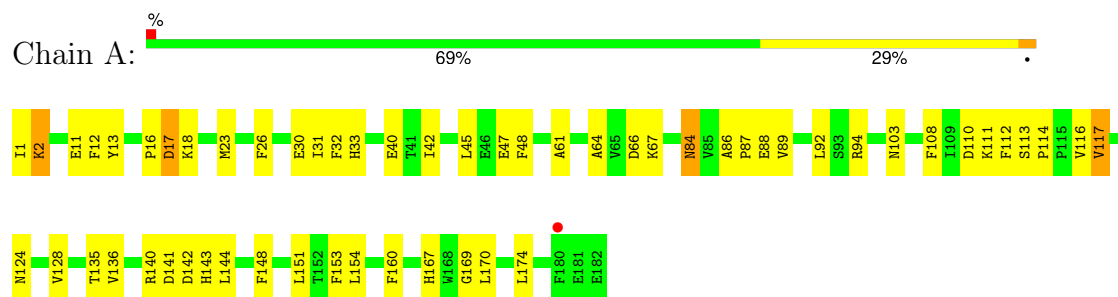
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total	O	0	0
			57	57		
5	B	51	Total	O	0	0
			51	51		
5	C	57	Total	O	0	0
			57	57		
5	D	50	Total	O	0	0
			50	50		

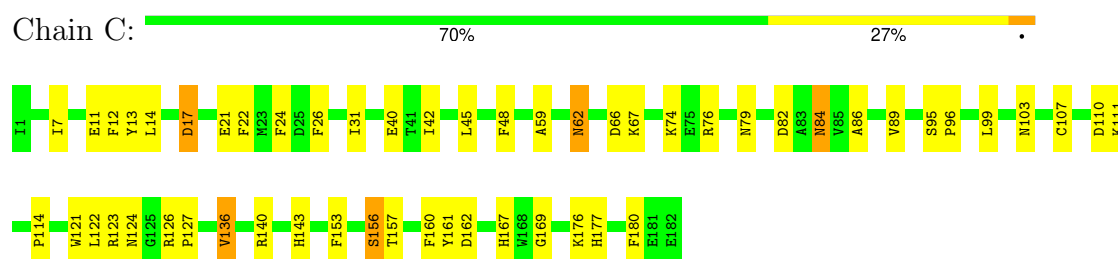
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

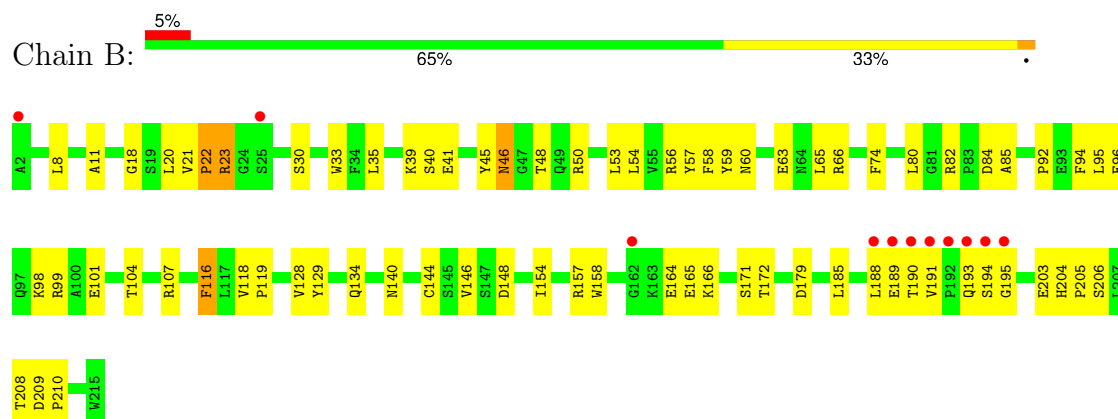
- Molecule 1: H-2 class II histocompatibility antigen, E-D alpha chain



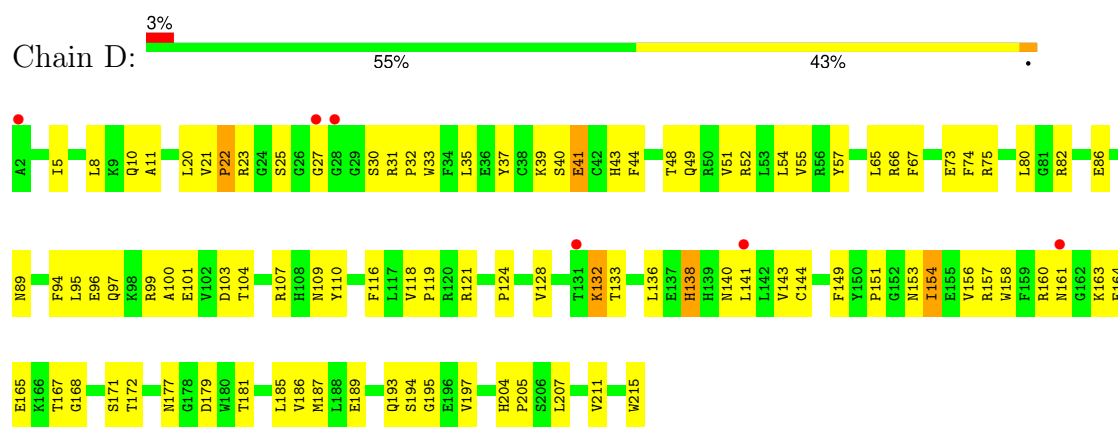
- Molecule 1: H-2 class II histocompatibility antigen, E-D alpha chain



- Molecule 2: Fusion protein consisting of cytochrome C peptide, glycine rich linker, and MHC E-beta-k



- Molecule 2: Fusion protein consisting of cytochrome C peptide, glycine rich linker, and MHC E-beta-k



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.79Å 56.93Å 115.99Å 90.00° 92.12° 90.00°	Depositor
Resolution (Å)	19.93 – 2.80 19.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.93-2.80) 92.8 (19.93-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.220 , 0.294 0.218 , 0.290	Depositor DCC
$R_{free}$ test set	1143 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.42	0/1543	0.66	0/2096
1	C	0.41	0/1543	0.65	0/2096
2	B	0.38	0/1768	0.64	0/2404
2	D	0.38	0/1768	0.68	1/2404 (0.0%)
All	All	0.40	0/6622	0.66	1/9000 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	133	THR	N-CA-C	-7.01	92.08	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1500	0	1421	52	0
1	C	1500	0	1422	46	0
2	B	1722	0	1640	57	0
2	D	1722	0	1640	87	0
3	E	28	0	25	1	0
4	A	28	0	26	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	14	0	13	0	0
4	D	14	0	13	2	0
5	A	57	0	0	1	0
5	B	51	0	0	0	0
5	C	57	0	0	1	0
5	D	50	0	0	1	0
All	All	6743	0	6200	223	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (223) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:VAL:HG22	2:D:187:MET:HG2	1.57	0.86
2:D:107:ARG:HG3	2:D:107:ARG:HH11	1.44	0.81
2:D:204:HIS:CD2	2:D:205:PRO:HD2	2.15	0.80
1:C:124:ASN:HA	1:C:160:PHE:CZ	2.17	0.80
2:D:8:LEU:HD22	2:D:40:SER:HB3	1.65	0.78
2:B:165:GLU:HG3	2:B:188:LEU:HD21	1.65	0.78
1:C:13:TYR:CE2	1:C:67:LYS:HG3	2.20	0.76
2:D:49:GLN:HE21	4:D:606:NAG:H82	1.51	0.74
1:C:84:ASN:N	1:C:84:ASN:HD22	1.86	0.73
1:C:157:THR:HG22	1:C:180:PHE:HD2	1.54	0.72
2:D:73:GLU:HB2	2:D:75:ARG:HH12	1.54	0.72
1:A:1:ILE:HG22	1:A:2:LYS:H	1.56	0.71
2:D:73:GLU:HB3	2:D:89:ASN:OD1	1.92	0.70
2:D:157:ARG:HD3	2:D:164:GLU:OE2	1.91	0.69
1:C:157:THR:HG22	1:C:180:PHE:CD2	2.28	0.69
2:D:49:GLN:NE2	4:D:606:NAG:H82	2.08	0.68
2:D:73:GLU:HB2	2:D:75:ARG:NH1	2.07	0.68
1:C:26:PHE:HB2	1:C:31:ILE:HD11	1.75	0.67
2:B:8:LEU:N	2:B:8:LEU:HD12	2.11	0.66
2:D:103:ASP:HA	2:D:107:ARG:HB2	1.77	0.66
2:D:54:LEU:HD11	2:D:66:ARG:HD3	1.78	0.65
1:A:167:HIS:H	1:A:170:LEU:HD12	1.63	0.64
2:D:96:GLU:OE2	2:D:99:ARG:NH1	2.31	0.64
2:D:163:LYS:HB2	2:D:163:LYS:NZ	2.12	0.63
2:D:141:LEU:CD2	2:D:189:GLU:HG2	2.28	0.63
1:A:84:ASN:HD22	1:A:84:ASN:N	1.97	0.62
2:D:121:ARG:HH11	2:D:121:ARG:HG3	1.65	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:204:HIS:HD2	2:D:205:PRO:HD2	1.61	0.61
1:C:22:PHE:CG	1:C:59:ALA:HB1	2.36	0.61
2:D:101:GLU:HA	2:D:104:THR:OG1	2.01	0.60
2:B:8:LEU:HD12	2:B:8:LEU:H	1.67	0.60
1:C:124:ASN:HA	1:C:160:PHE:CE2	2.37	0.59
2:D:163:LYS:HB2	2:D:163:LYS:HZ2	1.68	0.58
2:B:128:VAL:O	2:B:129:TYR:HB3	2.03	0.58
2:B:164:GLU:HG2	2:B:166:LYS:HG3	1.84	0.58
2:D:107:ARG:HH11	2:D:107:ARG:CG	2.12	0.58
2:B:190:THR:HG22	2:B:191:VAL:N	2.19	0.58
1:A:2:LYS:HD2	3:E:1:NAG:H82	1.86	0.57
1:C:99:LEU:HD21	1:C:157:THR:HG23	1.87	0.57
1:A:116:VAL:O	1:A:117:VAL:HG13	2.04	0.57
1:C:74:LYS:HE2	1:C:79:ASN:OD1	2.05	0.57
2:B:45:TYR:HB2	2:B:50:ARG:HB2	1.87	0.56
1:C:45:LEU:HD12	1:C:48:PHE:CZ	2.41	0.56
2:B:20:LEU:HD12	2:B:80:LEU:HD12	1.86	0.56
2:D:153:ASN:O	2:D:154:ILE:HB	2.05	0.56
1:A:111:LYS:HZ3	2:D:23:ARG:HE	1.54	0.56
2:D:141:LEU:HD21	2:D:189:GLU:HG2	1.88	0.56
2:B:56:ARG:HB3	2:B:63:GLU:OE2	2.06	0.55
2:B:98:LYS:HA	2:B:101:GLU:HG3	1.89	0.55
1:C:110:ASP:OD1	1:C:111:LYS:N	2.40	0.55
2:D:193:GLN:O	2:D:195:GLY:N	2.39	0.55
2:D:144:CYS:HB2	2:D:158:TRP:CZ2	2.41	0.55
2:D:164:GLU:HG3	2:D:165:GLU:N	2.22	0.55
2:B:157:ARG:HD3	2:B:164:GLU:OE2	2.07	0.54
2:D:48:THR:HG22	2:D:107:ARG:HD3	1.88	0.54
4:A:601:NAG:H83	4:A:601:NAG:O3	2.08	0.54
1:C:74:LYS:HB3	1:C:79:ASN:OD1	2.08	0.54
1:C:76:ARG:O	1:C:76:ARG:HG2	2.08	0.54
2:D:121:ARG:HG3	2:D:121:ARG:NH1	2.22	0.54
1:C:40:GLU:HG3	1:C:42:ILE:HD11	1.88	0.54
1:C:167:HIS:CD2	1:C:169:GLY:H	2.26	0.53
2:D:20:LEU:HD12	2:D:80:LEU:HD12	1.90	0.53
2:B:21:VAL:HG13	2:B:22:PRO:HD2	1.90	0.53
1:A:140:ARG:O	2:B:39:LYS:NZ	2.41	0.53
1:C:13:TYR:CD2	1:C:67:LYS:HG3	2.44	0.53
2:D:8:LEU:N	2:D:8:LEU:HD12	2.24	0.53
2:D:82:ARG:O	2:D:86:GLU:HG3	2.08	0.53
2:D:44:PHE:CZ	2:D:110:TYR:HB2	2.44	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.91	0.52
2:B:203:GLU:HG2	2:B:210:PRO:HG3	1.91	0.52
1:A:45:LEU:HD12	1:A:48:PHE:CZ	2.44	0.52
1:A:12:PHE:HB2	2:B:35:LEU:HD11	1.92	0.52
2:B:11:ALA:HB2	2:B:94:PHE:CZ	2.45	0.51
1:A:1:ILE:HG22	1:A:2:LYS:N	2.24	0.51
1:A:92:LEU:HD23	1:A:92:LEU:N	2.25	0.51
1:A:167:HIS:N	1:A:170:LEU:HD12	2.26	0.51
2:D:21:VAL:HG13	2:D:22:PRO:HD2	1.92	0.51
1:A:2:LYS:HA	2:B:46:ASN:OD1	2.10	0.51
2:D:151:PRO:HB2	5:D:610:HOH:O	2.09	0.51
2:D:103:ASP:OD1	2:D:107:ARG:NH1	2.43	0.51
2:B:128:VAL:HG12	2:B:129:TYR:N	2.25	0.51
2:D:119:PRO:O	2:D:121:ARG:HG2	2.11	0.51
1:A:88:GLU:OE2	2:D:25:SER:HB2	2.12	0.50
2:D:179:ASP:OD1	2:D:181:THR:OG1	2.26	0.50
1:A:2:LYS:HG3	2:B:46:ASN:OD1	2.12	0.50
1:A:13:TYR:CE2	1:A:67:LYS:HG3	2.47	0.50
2:B:53:LEU:HD12	2:B:54:LEU:N	2.27	0.50
1:C:84:ASN:N	1:C:84:ASN:ND2	2.55	0.50
2:D:11:ALA:HB2	2:D:94:PHE:CZ	2.46	0.50
2:D:172:THR:HG23	2:D:185:LEU:HB2	1.93	0.50
1:A:84:ASN:ND2	2:B:30:SER:HB3	2.26	0.50
2:D:107:ARG:CG	2:D:107:ARG:NH1	2.73	0.50
2:D:48:THR:CG2	2:D:107:ARG:HD3	2.42	0.49
2:B:59:TYR:O	2:B:60:ASN:HB2	2.13	0.49
1:C:86:ALA:HB2	1:C:169:GLY:O	2.12	0.49
1:C:99:LEU:HD21	1:C:157:THR:CG2	2.43	0.49
2:D:118:VAL:N	2:D:119:PRO:HD2	2.27	0.49
2:D:124:PRO:HB3	2:D:149:PHE:HB3	1.93	0.49
1:C:114:PRO:HB3	2:D:33:TRP:CE3	2.48	0.49
2:B:48:THR:HB	2:B:107:ARG:HD3	1.95	0.49
2:B:157:ARG:HG3	2:B:157:ARG:HH11	1.77	0.49
1:A:89:VAL:HG23	1:A:174:LEU:HD23	1.94	0.49
2:B:92:PRO:O	2:B:96:GLU:HG2	2.13	0.49
2:D:177:ASN:HB2	2:D:181:THR:O	2.12	0.49
1:A:124:ASN:HA	1:A:160:PHE:CZ	2.47	0.49
1:A:61:ALA:O	1:A:64:ALA:HB3	2.13	0.48
2:D:65:LEU:HD11	2:D:74:PHE:HB3	1.95	0.48
2:B:146:VAL:HG11	2:B:154:ILE:HD11	1.96	0.48
2:B:154:ILE:HG13	2:B:204:HIS:HB2	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:LEU:HD12	2:D:8:LEU:H	1.78	0.48
1:A:23:MET:HE1	1:A:30:GLU:HG3	1.96	0.48
2:D:171:SER:HA	2:D:185:LEU:O	2.14	0.48
1:A:114:PRO:HB3	2:B:33:TRP:CE3	2.49	0.48
2:B:63:GLU:CD	2:B:66:ARG:HH21	2.16	0.48
2:B:98:LYS:O	2:B:101:GLU:HG3	2.13	0.48
1:A:124:ASN:HA	1:A:160:PHE:CE2	2.48	0.47
1:A:86:ALA:HB2	1:A:169:GLY:O	2.14	0.47
2:D:51:VAL:HG12	2:D:52:ARG:N	2.30	0.47
1:A:108:PHE:CE2	1:A:110:ASP:HB2	2.49	0.47
2:B:65:LEU:HD11	2:B:74:PHE:HB3	1.96	0.47
2:B:95:LEU:O	2:B:99:ARG:HG3	2.14	0.47
2:B:154:ILE:HG13	2:B:203:GLU:O	2.14	0.47
1:A:114:PRO:HD3	2:B:33:TRP:CE2	2.50	0.47
2:B:8:LEU:HD22	2:B:40:SER:HB3	1.95	0.47
2:B:190:THR:HG22	2:B:191:VAL:H	1.78	0.47
1:A:33:HIS:CD2	1:A:136:VAL:HG11	2.49	0.47
2:B:157:ARG:HG3	2:B:157:ARG:NH1	2.29	0.47
1:C:12:PHE:CD1	1:C:12:PHE:C	2.88	0.47
2:D:41:GLU:HB2	2:D:43:HIS:NE2	2.29	0.47
2:D:65:LEU:HG	2:D:66:ARG:N	2.28	0.47
1:A:113:SER:HA	1:A:114:PRO:C	2.35	0.46
2:B:21:VAL:O	2:B:23:ARG:N	2.48	0.46
2:D:5:ILE:HG23	2:D:109:ASN:OD1	2.14	0.46
2:D:103:ASP:OD1	2:D:107:ARG:HG3	2.15	0.46
2:D:128:VAL:HG11	2:D:215:TRP:HB2	1.97	0.46
1:C:11:GLU:OE1	1:C:66:ASP:OD2	2.33	0.46
2:D:37:TYR:OH	2:D:39:LYS:HD3	2.15	0.46
1:A:88:GLU:OE1	1:A:111:LYS:NZ	2.49	0.46
2:D:107:ARG:HG3	2:D:107:ARG:NH1	2.23	0.46
1:C:103:ASN:HB3	1:C:153:PHE:CE1	2.51	0.46
2:B:57:TYR:HB2	2:B:65:LEU:HB3	1.98	0.46
2:B:116:PHE:CD1	2:B:116:PHE:N	2.83	0.46
2:B:144:CYS:HB2	2:B:158:TRP:CZ2	2.51	0.46
2:B:172:THR:HG22	2:D:21:VAL:HG21	1.97	0.46
2:D:20:LEU:CD1	2:D:80:LEU:HA	2.46	0.45
2:D:156:VAL:CG1	2:D:186:VAL:HG21	2.47	0.45
1:C:11:GLU:OE2	1:C:62:ASN:ND2	2.48	0.45
1:A:40:GLU:HG3	1:A:42:ILE:HD11	1.98	0.45
1:C:156:SER:OG	1:C:157:THR:N	2.50	0.45
1:A:12:PHE:CD1	1:A:12:PHE:C	2.90	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:HG11	1:A:151:LEU:HD11	2.00	0.44
1:A:110:ASP:OD1	1:A:111:LYS:N	2.46	0.44
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.83	0.44
1:C:123:ARG:HE	1:C:161:TYR:HE2	1.63	0.44
1:C:136:VAL:HG13	5:C:613:HOH:O	2.18	0.44
1:C:107:CYS:HB2	1:C:121:TRP:CH2	2.53	0.44
1:C:122:LEU:HB2	1:C:162:ASP:HB2	1.99	0.44
1:A:11:GLU:OE1	1:A:66:ASP:OD2	2.36	0.44
1:C:162:ASP:OD1	1:C:177:HIS:HA	2.18	0.44
1:A:31:ILE:HG22	1:A:32:PHE:HD1	1.83	0.44
2:D:207:LEU:HD13	2:D:211:VAL:HG23	1.99	0.44
2:B:193:GLN:C	2:B:195:GLY:H	2.21	0.43
2:D:156:VAL:HG11	2:D:186:VAL:HG21	2.00	0.43
2:D:168:GLY:O	2:D:189:GLU:HG3	2.18	0.43
1:C:11:GLU:HA	1:C:21:GLU:O	2.17	0.43
1:A:23:MET:CE	1:A:30:GLU:HG3	2.47	0.43
1:A:92:LEU:HD23	1:A:92:LEU:H	1.82	0.43
1:A:103:ASN:HB3	1:A:153:PHE:CE1	2.53	0.43
2:B:20:LEU:HD12	2:B:80:LEU:HA	2.01	0.43
2:D:21:VAL:CG1	2:D:22:PRO:HD2	2.48	0.43
2:D:153:ASN:O	2:D:204:HIS:HD2	2.01	0.43
1:C:143:HIS:CD2	1:C:143:HIS:H	2.36	0.43
2:D:116:PHE:N	2:D:116:PHE:CD1	2.87	0.43
2:D:97:GLN:O	2:D:100:ALA:N	2.52	0.43
2:D:207:LEU:HD13	2:D:211:VAL:CG2	2.47	0.43
1:A:111:LYS:NZ	2:D:23:ARG:HE	2.16	0.42
1:A:135:THR:HG23	1:A:148:PHE:HB2	2.01	0.42
2:B:21:VAL:CG1	2:B:22:PRO:HD2	2.49	0.42
2:B:118:VAL:N	2:B:119:PRO:HD2	2.34	0.42
1:C:66:ASP:OD1	2:D:10:GLN:OE1	2.37	0.42
2:B:148:ASP:CG	2:B:148:ASP:O	2.57	0.42
2:B:189:GLU:O	2:B:190:THR:OG1	2.32	0.42
1:C:14:LEU:HD13	2:D:35:LEU:HB2	2.02	0.42
1:C:45:LEU:HB2	1:C:48:PHE:CE2	2.54	0.42
2:D:44:PHE:HD1	2:D:51:VAL:HG22	1.85	0.42
2:D:149:PHE:HB2	2:D:204:HIS:CE1	2.55	0.42
1:A:143:HIS:CE1	1:A:144:LEU:HD21	2.54	0.42
1:C:7:ILE:HD12	2:D:44:PHE:HE2	1.84	0.42
2:D:167:THR:HG22	2:D:168:GLY:N	2.34	0.42
1:A:17:ASP:O	1:A:18:LYS:HB2	2.19	0.42
1:A:87:PRO:HB3	1:A:112:PHE:CD1	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LYS:HE2	1:C:74:LYS:HB3	1.89	0.42
1:C:114:PRO:HD3	2:D:33:TRP:CE2	2.55	0.42
1:C:89:VAL:HG12	1:C:176:LYS:HG3	2.01	0.42
1:C:124:ASN:HA	1:C:160:PHE:CE1	2.54	0.42
1:C:126:ARG:HA	1:C:127:PRO:HD3	1.93	0.42
1:A:84:ASN:N	1:A:84:ASN:ND2	2.66	0.42
1:A:111:LYS:HE2	2:D:23:ARG:HH21	1.85	0.42
1:C:84:ASN:ND2	2:D:30:SER:HB3	2.35	0.42
1:C:140:ARG:O	2:D:39:LYS:NZ	2.51	0.42
2:D:95:LEU:HD13	2:D:99:ARG:NH2	2.35	0.42
2:D:161:ASN:HB2	2:D:163:LYS:HE3	2.01	0.42
1:A:47:GLU:HG2	5:A:652:HOH:O	2.19	0.41
2:B:204:HIS:HE1	2:B:206:SER:HB3	1.85	0.41
1:A:16:PRO:O	1:A:18:LYS:HG3	2.20	0.41
2:D:31:ARG:HA	2:D:32:PRO:HD3	1.95	0.41
2:D:57:TYR:CD2	2:D:65:LEU:HD23	2.55	0.41
2:D:197:VAL:O	2:D:197:VAL:HG13	2.19	0.41
1:A:94:ARG:NE	2:B:179:ASP:OD2	2.50	0.41
2:D:95:LEU:HD23	2:D:95:LEU:HA	1.94	0.41
2:D:97:GLN:O	2:D:100:ALA:HB3	2.20	0.41
1:A:1:ILE:O	1:A:2:LYS:HB2	2.21	0.41
1:A:47:GLU:HG2	1:A:47:GLU:H	1.67	0.41
2:B:41:GLU:HG3	2:B:54:LEU:O	2.21	0.41
2:B:101:GLU:HA	2:B:104:THR:OG1	2.21	0.41
2:D:55:VAL:HB	2:D:67:PHE:HB3	2.03	0.41
2:B:171:SER:HA	2:B:185:LEU:O	2.20	0.40
2:B:209:ASP:O	2:B:210:PRO:C	2.60	0.40
2:B:65:LEU:HD22	2:B:84:ASP:HB2	2.03	0.40
2:B:82:ARG:O	2:B:85:ALA:N	2.54	0.40
2:B:58:PHE:CE2	2:B:63:GLU:HB2	2.56	0.40
1:C:89:VAL:O	1:C:176:LYS:HE3	2.21	0.40
1:C:95:SER:HB2	1:C:96:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/182 (99%)	164 (91%)	14 (8%)	2 (1%)	12	37
1	C	180/182 (99%)	164 (91%)	14 (8%)	2 (1%)	12	37
2	B	211/213 (99%)	181 (86%)	22 (10%)	8 (4%)	2	9
2	D	211/213 (99%)	180 (85%)	24 (11%)	7 (3%)	3	11
All	All	782/790 (99%)	689 (88%)	74 (10%)	19 (2%)	5	18

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	23	ARG
2	D	136	LEU
2	D	194	SER
2	B	18	GLY
2	B	46	ASN
2	B	140	ASN
1	A	2	LYS
1	A	142	ASP
2	B	22	PRO
2	B	194	SER
2	D	27	GLY
1	C	17	ASP
2	D	132	LYS
2	B	134	GLN
2	B	205	PRO
2	D	138	HIS
2	D	22	PRO
2	D	154	ILE
1	C	136	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/165 (100%)	161 (98%)	4 (2%)	44	77
1	C	165/165 (100%)	159 (96%)	6 (4%)	30	64
2	B	189/189 (100%)	187 (99%)	2 (1%)	70	90
2	D	189/189 (100%)	184 (97%)	5 (3%)	41	75
All	All	708/708 (100%)	691 (98%)	17 (2%)	44	77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	84	ASN
1	A	117	VAL
1	A	141	ASP
2	B	116	PHE
2	B	208	THR
1	C	17	ASP
1	C	24	PHE
1	C	62	ASN
1	C	82	ASP
1	C	84	ASN
1	C	156	SER
2	D	41	GLU
2	D	132	LYS
2	D	138	HIS
2	D	140	ASN
2	D	160	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	167	HIS
1	A	177	HIS
2	B	10	GLN
1	C	84	ASN
1	C	143	HIS
1	C	167	HIS
2	D	10	GLN
2	D	49	GLN
2	D	201	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	E	1	3,2	14,14,15	0.70	0	17,19,21	0.75	0
3	NAG	E	2	3	14,14,15	0.60	0	17,19,21	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	1/1/5/7	5/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	NAG	C1

All (7) torsion outliers are listed below:

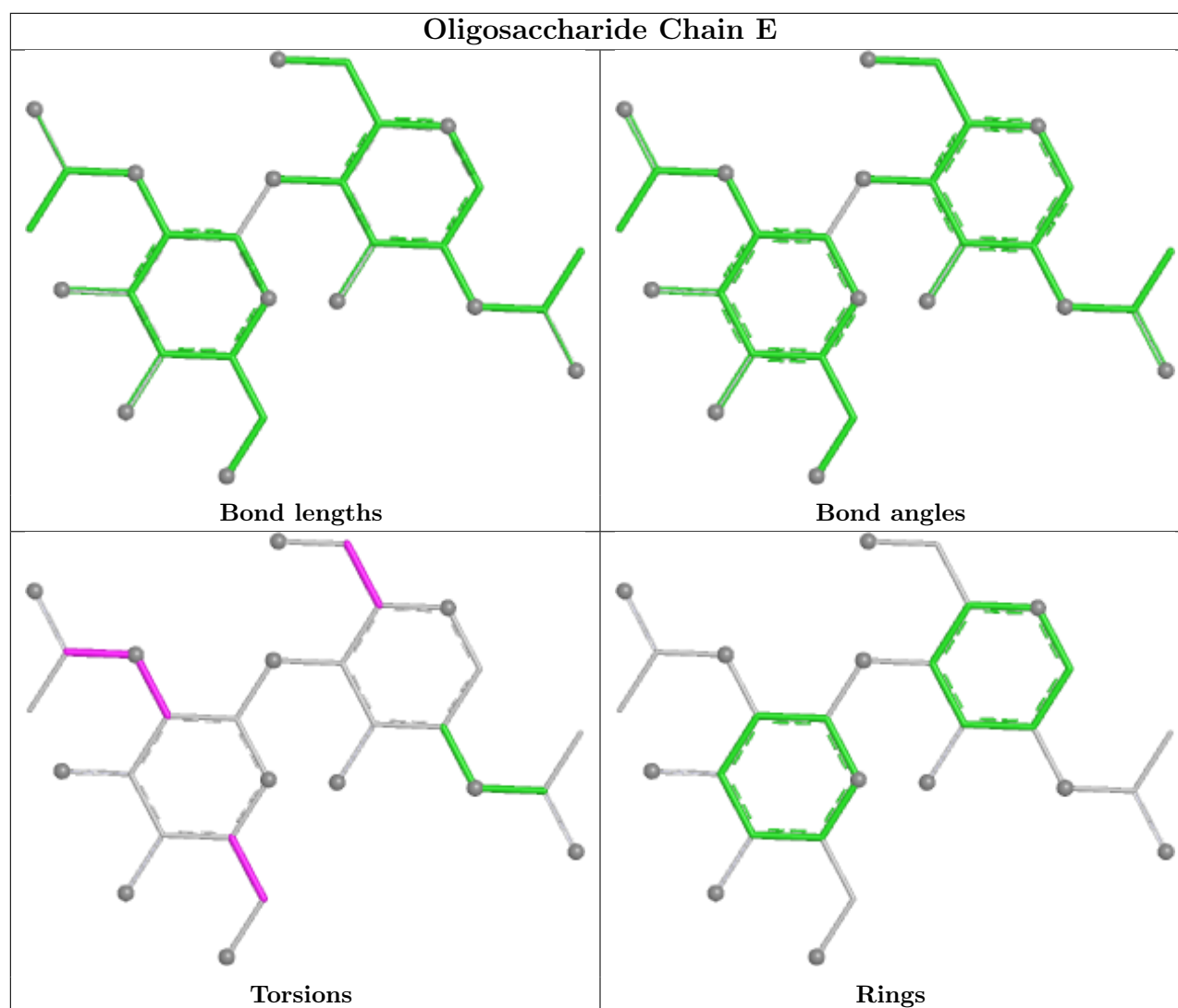
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	602	1	14,14,15	0.69	0	17,19,21	0.70	0
4	NAG	C	605	1	14,14,15	0.62	0	17,19,21	0.67	0
4	NAG	D	606	2	14,14,15	0.79	1 (7%)	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	601	1	14,14,15	0.59	0	17,19,21	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	602	1	-	3/6/23/26	0/1/1/1
4	NAG	C	605	1	-	2/6/23/26	0/1/1/1
4	NAG	D	606	2	-	3/6/23/26	0/1/1/1
4	NAG	A	601	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	606	NAG	C1-C2	2.38	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
4	A	602	NAG	C8-C7-N2-C2
4	A	602	NAG	O7-C7-N2-C2
4	C	605	NAG	C8-C7-N2-C2
4	C	605	NAG	O7-C7-N2-C2
4	D	606	NAG	C8-C7-N2-C2
4	D	606	NAG	O7-C7-N2-C2
4	D	606	NAG	O5-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	A	602	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	606	NAG	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	182/182 (100%)	-0.49	1 (0%) 87 83	13, 35, 61, 151	0
1	C	182/182 (100%)	-0.56	0 100 100	15, 33, 65, 110	0
2	B	201/213 (94%)	-0.05	11 (5%) 32 25	21, 42, 119, 170	0
2	D	204/213 (95%)	-0.17	6 (2%) 54 45	17, 39, 104, 142	0
All	All	769/790 (97%)	-0.31	18 (2%) 61 52	13, 37, 98, 170	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	194	SER	4.6
2	B	191	VAL	4.5
2	B	193	GLN	3.9
2	D	2	ALA	3.3
2	B	189	GLU	3.0
1	A	180	PHE	2.8
2	B	188	LEU	2.8
2	B	25	SER	2.7
2	D	141	LEU	2.6
2	B	195	GLY	2.5
2	D	131	THR	2.5
2	B	192	PRO	2.4
2	B	190	THR	2.3
2	D	161	ASN	2.2
2	B	2	ALA	2.1
2	D	27	GLY	2.1
2	B	162	GLY	2.1
2	D	28	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

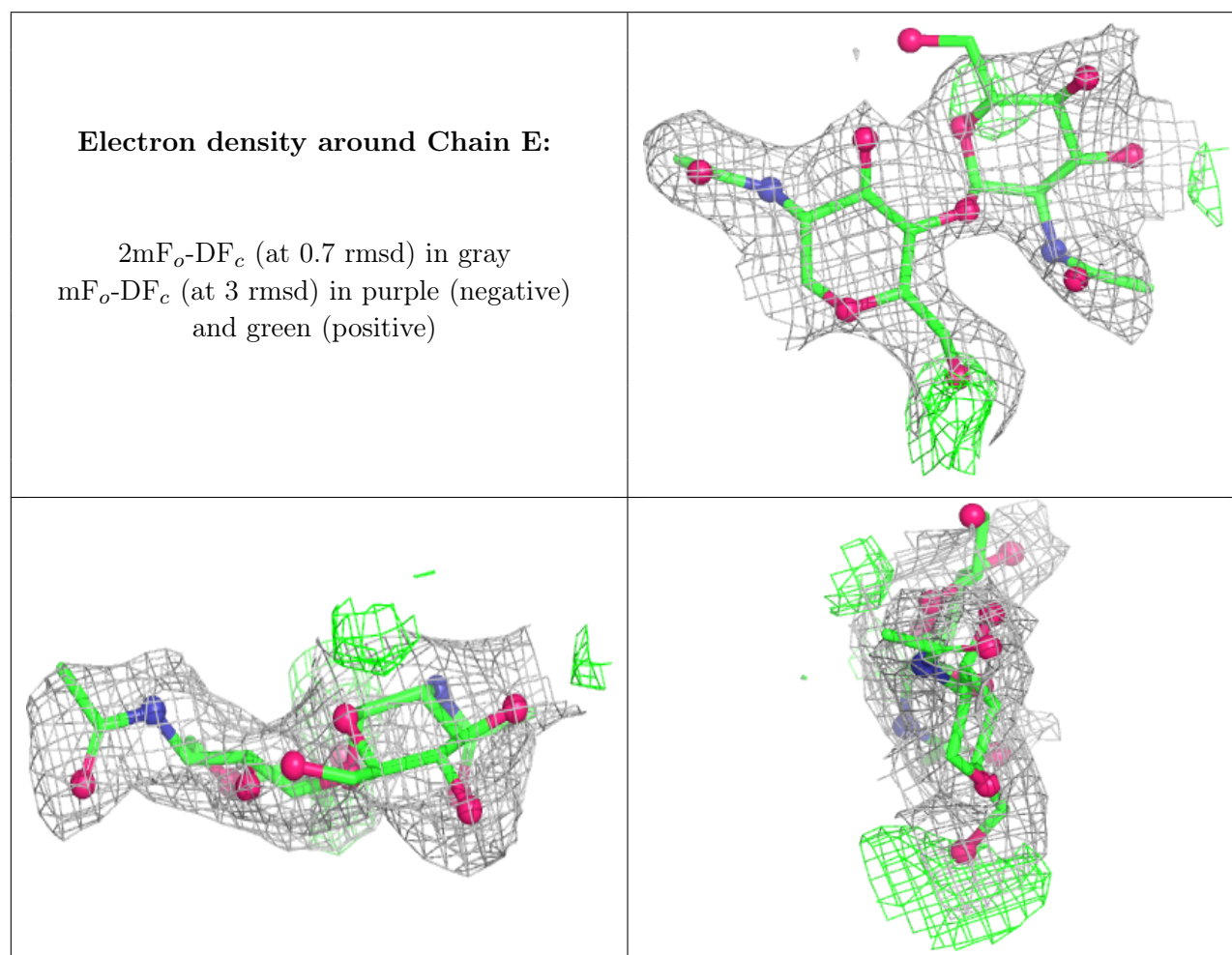
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	1	14/15	0.64	0.14	59,61,65,69	0
3	NAG	E	2	14/15	0.72	0.13	73,76,77,78	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	601	14/15	0.47	0.16	101,107,108,108	0
4	NAG	C	605	14/15	0.69	0.11	63,66,70,72	0
4	NAG	D	606	14/15	0.73	0.12	55,58,58,59	0
4	NAG	A	602	14/15	0.82	0.12	71,76,79,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.